Modeling, Algorithms, and Informatics (CCS-3)
Publications and Presentations, March 2004 to March 2005

Refereed/Peer Journals

F. Alexander, G. Eyink, and J. Restrepo, "Accelerated Monte-Carlo for Optimal Estimation of Time Series," *Journal of Statistical Physics*, 2004, to appear.

F. Alexander, A. Garcia, and D. Tartakovsky, "Algorithm Refinement for Stochastic Partial Differential Equations: II Correlated Systems," *Journal of Computational Physics*, 2004, to appear.

F. Alexander, A. Garcia, and D. Tartakovsky, "Noise in Algorithm Refinement Methods," *Computing in Science and Engineering*, to appear 2005.

M. Anghel, Y. Ben-Zion, and R. Rico-Martinez, "Dimensional Reduction, Nonlinear System Identification and Forecasting of Earthquake Fault Dynamics," *Pure and Applied Geophysics*, 161, 2023-2051, 2004.

L. Arber and S. Pakin, "The Impact of Message-Buffer Alignment on Communication Performance," *Parallel Processing Letters*, to appear in June 2005. (Also a technical report, LA-UR-04-6066, Los Alamos National Laboratory.) Available from http://www.c3.lanl.gov/~pakin/papers/ppl2005.pdf.

J. Beecroft, D. Addison, D. Hewson, M. McLaren, F. Petrini, and D. Roweth, "Quadrics QsNet II: Pushing the Limit of the Design of High-Performance Networks for Supercomputers," *IEEE Micro*, to appear in 2005.

A. Christmann and I. Steinwart, "On Robustness Properties of Convex Risk Minimization Methods for Pattern Recognition," *Journal of Machine Learning Research*, 5:1007-1034, 2004.

G. Eyink, J. Restrepo, and F. Alexander, "A Mean-Field Approximation in Data Assimilation for Nonlinear Dynamics," *Physica D*, to appear.

G. Eyink, J. Restrepo, and F. Alexander, "A Statistical-Mechanical Approach to Data Assimilation for Nonlinear Dynamics: II. Evolution Approximations," submitted to the *Journal of Statistical Physics*, 2004.

S. Ferson, C. Joslyn, J. Helton, W. Oberkampf, and K. Sentz, "Summary of the Epistemic Uncertainty Workshop: Consensus Amid Diversity," *Reliability Engineering and Systems Safety*, Vol. 85:1-3, pp. 355-370, 2004.

E. Frachtenberg, D. Feitelson, F. Petrini, and J. Fernandez, "Adaptive Parallel Job Scheduling with Flexible Co-Scheduling," in *IEEE Transactions on Parallel and Distributed Systems*, to appear 2005.

L. Guo, S. Jiang, L. Xiao, and X. Zhang, “Fast and Low Cost P2P Searching by Exploiting Localities in Peer Community and Individual Peers,” *Journal of Parallel and Distributed Computing*, to appear 2005.

M. Guo, L. Yang, M. Buecker, J. Cao, W. Chang, V. Chaudhary, B. Di Martino, W. Jia, D. Kerbyson, J. Li, T. Rauber, and G. Runga (editors), "Hardware/Software Support for High Performance Scientific and Engineering Computing," *IEICE Transactions on Information Systems*, Vol. 87, July 2004.

L.Gurvits, “Classical Complexity and Quantum Entanglement,” *Journal of Computer and System Sciences*, 2004.

L.Gurvits, “Combinatorial and Algorithmic Aspects of Hyperbolic Polynomials,” *Electronic Colloquium on Computational Complexity*, Volume 11, 2004.

L. Gurvits, “The Van der Waerden Conjecture for Mixed Discriminants,” *Advances in Mathematics*, in press, 2005.

L.Gurvits and J. Ledoux, “Markov Property for a Function of a Markov Chain: A Linear Algebra Approach,” *Linear Algebra and its Applications*, in press, 2005.

L. Gurvits and L. Rodman, “On Matrix Polynomials with Real Roots,” *SIAM Journal of Matrix Analysis*, Vol. 26, No. 3, pp. 758-764, 2005.

D. Hush and C. Scovel, “Fat-Shattering of Affine Functions,” *Combinatorics Probability and Computing*, Vol. 13, pp. 353-360, 2004.

S. Jiang and X. Zhang, “Making LRU Friendly to Weak Locality Workloads: A Novel Replacement Algorithm to Improve File Buffer Cache Performance,” *IEEE Transactions on Computers*, to appear 2005.

S. Jiang and X. Zhang, “Token-Ordered LRU: An Efficient Page Replacement Policy and Implementation in Linux Systems,” in *Performance Evaluation*, 60 (1-4): 5-29. To appear May 2005.

C. Joslyn, S. Mniszewski, A. Fulmer, and G. Heaton, “The Gene Ontology Categorizer," *Bioinformatics*, Vol. 20:s1, pp. 169-177, 2004.

D. Kerbyson, A. Hoisie, S.Pakin, F. Petrini, and H. Wasserman, “A Performance Evaluation of an Alpha EV7 Processing Node,” the *International Journal of High Performance Computing Applications*, 18(2):199-209, May 1, 2004. (Available from http://www.c3.lanl.gov/~pakin/papers/ijhpca_ev7.pdf.)

D. Martin, P. Colella, M. Anghel, and F. Alexander, “Adaptive Mesh Refinement for Multiscale Nonequilibrium Physics,” *Computers in Science and Engineering*, in press. (Also a technical report, LA-UR-05-0749, Los Alamos National Laboratory.)

D. Martin, P. Colella, M. Anghel, and F. Alexander, “Adaptive Mesh Refinement for Multiscale Nonequilibrium Physics,” *Computing in Science and Engineering*, to appear in 2005.

W. Oberkampf, J. Helton, C. Joslyn, S. Wojtkiewicz, and S. Ferson, “Uncertainty in System Response Given Uncertain Parameters," *Reliability Engineering and System Safety*, Vol. 85:1-3, pp.~11-20, 2004.

M. Pernice and R. Hornung, "Newton-Krylov-FAC Methods for Problems Discretized on Locally Refined Grids," *Computing and Visualization in Science*, to appear in 2005.

F. Petrini, J. Fernandez, A. Moody, E. Frachtenberg, and D. Panda, “NIC-based Reduction Algorithms for Large-Scale Clusters,” *International Journal of High Performance Computing and Networking*, to appear 2005.

I. Steinwart, D. Hush, and C. Scovel, “A Classification Framework for Anomaly Detection,” *Journal of Machine Learning Research*, 6:211-232, 2005.

I. Steinwart, “Consistency of Support Vector Machines and other Regularized Kernel Machines,” *IEEE Transactions on Information Theory*, 51:128-142, 2005.

I. Steinwart, “Entropy of Convex Hulls—Some Lorentz Norm Results,” *Journal of Approximation Theory*, 128:42-52, 2004.

K. Summers, T. Caudell, K. Berkbigler, B. Bush, K. Davis, and S. Smith, “Graph Visualization for the Analysis of the Structure and Dynamics of Extreme-Scale Supercomputers,” *Information Visualization,* 3, pp. 209-222, 2004.

B. Uberuaga, M. Anghel, and A. Voter, “Synchronization of Trajectories in Canonical Molecular Dynamics Simulations,” *Journal of Chemical Physics*, 120, 6363, 2004.

K. Verspoor, “Toward a Semantic Lexicon for Biological Language Processing,” *Comparative and Functional Genomics*, Vol. 6, issue 1-2, pp. 61-66. DOI: 10.1002/cfg.451.

K. Verspoor, J. Cohn, C. Joslyn, S. Mniszewski, A. Rechtsteiner, L. Rocha, and T. Simas, “Protein Annotation as Term Categorization in the Gene Ontology Using Word Proximity Networks,” *BMC Bioinformatics*, to appear in 2005.

T. Warnock, R. Nemzek, J. Dreicer, and D. Torney, “Distributed Sensor Networks for Detection of Mobile Radioactive Sources,” *IEEE Transactions on Nuclear Science,* 51, pp. 1693-1700, August 2004.

C. Winter, E. Springer, K. Costigan, P. Fasel, S. Mniszewski, and G. Zyvoloski, "Virtual Watersheds: Simulating the Water Balance of the Rio Grande Basin," *IEEE Computers in Science and Engineering*, Vol. 6, Number 3, pp. 18-26, May/June 2004.

Technical Reports

K. Atkins, C. Barrett, J. Cohn, C. Homan, S. Kothapally, A. Marathe, M. Marathe., S. Mniszewski, and P. Romero, Marketecture Version 2.0, June 2004.

K. Atkins, J. Cohn, C. Homan, S. Kothapally, A. Marathe, and S. Mniszewski, Urban Infrastructure Suite: Financial/Energy Sector, Marketecture: Chicago Case Study, May 2004.

K. Berkbigler, et. al., Urban Population Mobility Simulation Technologies Volume 4: Population Generation, technical documentation, also in LA-UR-04-6039, Los Alamos National Laboratory.

M. Cannon and T. Warnock, "A Shape Descriptor Based on the Line Scan Transform," a technical report, LA-UR-04-5865, Los Alamos National Laboratory.

M. Cannon, T. Warnock, and S. Kumar, "A New Shape Metric Based on the Line Scan Transform (U)," technical report, LA-UR-04-3931, Los Alamos National Laboratory.

A. Christmann and I. Steinwart, "Consistency and Robustness of Kernel Based Regression," a technical report, LA-UR 04-8797, Los Alamos National Laboratory. Submitted to *Annals of Statistics*.

K. Davis, A. Hoisie, G. Johnson, D. Kerbyson, M. Lang, S. Pakin, and F. Petrini, "Lightning: A Performance and Scalability Report on the Use of 1020 Nodes," technical report, LA-UR-04-1652, Los Alamos National Laboratory.

K. Davis, A. Hoisie, G. Johnson, D. Kerbyson, M. Lang, S. Pakin, and F. Petrini, "Lightning: Performance Results for the Level 2 Milepost," technical report, LA-UR-04-5064, Los Alamos National Laboratory.

E. Frachtenberg. "Process Coordination for Commodity Systems," a technical report, LA-UR-04-7256, Los Alamos National Laboratory, December 2004.

A. Hoisie and S. Pakin, "Performance Modeling of a 2010-era ASC Supercomputer (U)," internal report, LA-CP-05-0172, Los Alamos National Laboratory.

G. Johnson, M. Lang, and D. Kerbyson, "Empirical Analysis of Various Memory Models on an Intel EM64T Based Processing Node," technical report, LA-UR-04-7449, Los Alamos National Laboratory.

C. Joslyn, “A Formerly Breathless Introduction to Generalized Information Theory," technical report, LA-UR-04-4078, Los Alamos National Laboratory, ftp://ftp.c3.lanl.gov/pub/users/joslyn/shortcourse.pdf .

C. Joslyn, “GIT Analysis of the Crushable Foam Experiment and Simulations," technical report, LA-UR-04-6207, Los Alamos National Laboratory, ftp://ftp.c3.lanl.gov/pub/users/joslyn/foam.pdf .

C. Joslyn, J. Oliverira, and C. Scherrer, “Order Theoretical Knowledge Discovery: A White Paper," technical report, LA-UR-04-5812, Los Alamos National Laboratory, ftp://ftp.c3.lanl.gov/pub/users/joslyn/white.pdf .

C. Joslyn, K. Verspoor, S.Mniszewski, and J. Cohn, “Automated Protein Function Annotation via Markov Adjusted Ontology Categorization,” a technical report, LA-UR-05-0639, Los Alamos National Laboratory.

D. Kerbyson, “A Note on the Different Task Mappings of SAGE onto BG/L,” technical report, LA-UR-04-4118, Los Alamos National Laboratory.

D. Kerbyson, “An Initial Analysis of Application Communication Degree,” technical report, LA-UR-04-7456, Los Alamos National Laboratory.

D. Kerbyson, “Discussion Document 1: Modeling the PERCS Networks,” internal report, LA-CP-04-0941, Los Alamos National Laboratory.

D. Kerbyson and K. Barker, “Automatic Identification of Application Communication Patterns via Templates,” technical report, LA-UR-04-7451, Los Alamos National Laboratory.

D. Kerbyson and A. Hoisie, “An Initial Analysis of the BG/P System,” technical report, LA-UR-04-5140, Los Alamos National Laboratory.

D. Kerbyson, M. Lang, G. Johnson, "A Note on the Performance of the EM64T (Nacona) Node,” technical report, LA-UR-04-7450, Los Alamos National Laboratory.

D. Kerbyson and P. Jones, “An Initial Performance Model of POP,” technical report, LA-UR-04-4119, Los Alamos National Laboratory.

D. Kerbyson and P. Jones, “A Performance Model of the Parallel Ocean Program,” technical report, LA-UR-04-8793, Los Alamos National Laboratory.

D. Kerbyson and M. Lang, “An Initial Performance Analysis of Commodity Memories in Intel Processing Nodes,” technical report, LA-UR-04-2111, Los Alamos National Laboratory.

M. Mathis and D. Kerbyson, “A General Performance Model of Structured and Unstructured Mesh Particle Transport Computations,” technical report, LA-UR-04-8794, Los Alamos National Laboratory.

S. Mniszewski, “POset Ontology Categorizer (POSOC) Software Design Notes,” included with the POSOC Open Source Distribution, technical report, LA-UR-04-8799, Los Alamos National Laboratory.

M. Pernice and B. Philip, “Solution of Equilibrium Radiation Diffusion Problems Using Implicit Adaptive Mesh Refinement,” technical report, LA-UR-04-3620, Los Alamos National Laboratory.

C. Scovel, D. Hush, and I. Steinwart, “Learning Rates for Density Level Detection,” a technical report, submitted for publication as a technical report (an LA-UR in 2005), at Los Alamos National Laboratory.

D. Spooner and D. Kerbyson, “Performance Feature Identification by Comparative Analysis,” technical report, LA-UR-04-7522, Los Alamos National Laboratory.

I. Steinwart, D. Hush, and C. Scovel, “An Explicit Description of the Reproducing Kernel Hilbert Spaces of Gaussian RBF Kernels,” a technical report, LA-UR 04-8274, Los Alamos National Laboratory. Submitted to *IEEE Transactions on Information Theory*.

I. Steinwart and C. Scovel, “Fast Rates for Support Vector Machines,” a technical report, LA-UR 05-0451, Los Alamos National Laboratory. Submitted to the Conference on Learning Theory.)

I. Steinwart and C. Scovel, “Fast Rates for Support Vector Machines Using Gaussian Kernels,” a technical report, LA-UR 04-8796, Los Alamos National Laboratory. Submitted to *Annals of Statistics*.

K. Verspoor, C. Joslyn, J. Ambrosiano, A. Backer, O. Bodenreider, L. Hirschman, P. Karp, H. Kelly, S. Loranger, M. Musen, R. Sriram, and C. Wroe, “Knowledge Integration for Biothreat Response,” technical report, LA-UR-05-0907, Los Alamos National Laboratory.

Book Chapters/Edited Books/Book Reviews

A. Christmann and I. Steinwart, "Support Vector Machines: Theory and Applications," a book in preparation for Springer, New York, N.Y.

J. Fernandez, F. Petrini, E. Frachtenberg, "Achieving Predictable and Scalable Performance with BCS-MPI," in Engineering the Grid: Status and Perspective, B. Di Martino, J. Dongarra, A. Hoisie, L. Yang, H. Zima (editors), to appear 2005.

C. Joslyn, "Poset Ontologies and Concept Lattices as Semantic Hierarchies," in Conceptual Structures at Work, Lecture Notes in Artificial Intelligence, Vol. 3127, Wolff, Pfeiffer, and Delugach (editors), pp. ~287-302, Springer-Verlag, Berlin.

C. Joslyn and J. Booker, "Generalized Information Theory for Engineering Modeling and Simulation," in Engineering Design Reliability Handbook, E. Nikolaidis et al. (editors), pp. 9:1-40, CRC Press.

C. Joslyn and W. Bruno, "Weighted Pseudo-Distances for Categorization in Semantic Hierarchies," to appear in 2005 International Conference on Conceptual Structures, Lecture Notes in Artificial Intelligence.

Conference Proceedings, Talks, Etc.

M. Anghel, "A Bayesian Contribution to Performance Modeling," invited talk given at the Fifth Symposium of the Los Alamos Computer Science Institute: LACSI 2004, October 12-14, Santa Fe, N.M. (Also, a technical report, LA-UR-04-7199, Los Alamos National Laboratory.)

M. Anghel, S. Mniszewski, D. Kerbyson, and F. Alexander, "A Bayesian Contribution to Performance Analysis," Los Alamos Computer Science Institute Symposium (LACSI 2004), Workshop on Performance and Productivity of Extreme-Scale Parallel Systems, October 2004.

S. Boettcher, G. Istrate, and A.G. Percus, "Spines of Random Constraint Satisfaction Problems: Definition and Impact on Computational Complexity," in Proceedings of the Eighth International Symposium on Artificial Intelligence and Mathematics (AIMATH '04), AI&M 2-2004. Also to appear in 2005 in *Annals of Mathematics and Artificial Intelligence.*

S. Boettcher and A. Percus, "Extremal Optimization at the Phase Transition of the 3-Coloring Problem," *Physical Review E* 69, 066703, 2004.

A. Cannon and D. Hush, "Multiple-Instance Learning with Simple Classifiers," submitted and accepted for publication in ICMLA-2004 (for the 2004 International Conference on Machine Learning Applications).

J. Cohn, C. Joslyn, S. Mniszewski, and K. Verspoor, "Making the CASP Functional Annotation Process into a Widget," PFIG meeting, February 2005.

J. Cohn, C. Joslyn, S. Mniszewski, and K. Verspoor, "Predicting Protein Function Using Nearest Neighbor Categorization," poster at Bioscience Division Review, March 2005.

J. Cohn, K. Verspoor, S. Mniszewski, and C. Joslyn, "Predicting Protein Function Using Nearest Neighbor Categorization," poster at Second Annual Rocky Mountain Regional Bioinformatics Conference, December 2004.

K. Davis, A. Hoisie, G. Johnson, D. Kerbyson, M. Lang, S. Pakin, and F. Petrini, "A Performance and Scalability Analysis of the BlueGene/L Architecture," in Proceedings of SuperComputing (SC2004), Pittsburgh, Pa., November 6-12, 2004. (Also, a technical report, LA-UR-04-5620, Los Alamos National Laboratory.) Available at: http://www.sc-conference.org/sc2004/schedule/pdfs/pap302.pdf.

K. Davis and F. Petrini, "Achieving Usability and Efficiency in Large-Scale Parallel Computing Systems (Tutorial)," Europar 2004, Pisa, Italy.

K. Eggert, E. Beighley, T. Dunne, L. Mertes, K. Verdin, K., and S. Mniszewski, "Application of a Continental Scale River Modeling Framework to the Purus River Basin–A Major Tributary of the Amazon River," NCAR CCSM Land Working Group Meeting, March 2005.

K. Eggert, E. Beighley, T. Dunne, K. Verdin, and S. Mniszewski, "A Continental Scale River Modeling Framework Designed around Topographic Modeling Units with Both Hydrologic and Hydraulic Realism," NCAR Ninth Annual CCSM Workshop, July 2004.

E. Frachtenberg. "Designing Parallel Operating Systems Using Modern Interconnects," in Computer Science and Artificial Intelligence Laboratory (CSAIL), Massachusetts Institute of Technology, Cambridge, Mass., September 2004.

E. Frachtenberg. "Toward Realistic Evaluation of Job Scheduling Strategies," in a seminar talk, given at the Computer Science Departments of Hebrew University (Jerusalem), Tel Aviv University (Tel Aviv), Technion, Israel Institute of Technology (Haifa), Interdisciplinary Center (Herzlia), and Ben Gurion University, (Beer Sheva), Israel, December 2004.

E. Frachtenberg. "Using Multi-Rail Networks in High-Performance Clusters," in ClubNet, Department of Electrical Engineering, Technion Israel Institute of Technology, Haifa, Israel, December 2004.

R. Gioiosa, F. Petrini, K. Davis, and F. Lebaillif-Delamare, "Analysis of System Overhead on Parallel Computers," in the Fourth IEEE International Symposium on

Signal Processing and Information Technology (ISSPIT 2004), Rome, Italy, December 2004.

N. Gulbahce, F. Alexander, G. Johnson, “A Space-Time Cluster Monte Carlo Algorithm for Optimal Estimation,” in preparation.

N. Gulbahce, W. Klein, and H. Gould, “Heterogeneity in Classical and Non-Classical Nucleation,” cond-mat/0407304.

L. Guo, S. Jiang, L. Xiao, and X. Zhang, “Exploiting Content Localities for Efficient Search in P2P Systems,” in Proceedings of the 18th International Symposium on Distributed Computing DISC'04, Amsterdam, Netherlands, October 2004.

L. Gurvits, “Algebraic, Combinatorial and Geometric Properties of Quantum Entanglement,” 16th International Symposium on Mathematical Theory of Networks and Systems, Belgium, 2004.

L. Gurvits, “Combinatorial and Algorithmic Aspects of Hyperbolic Polynomials,” Brooklyn Poly, October 2004.

L. Gurvits, “Combinatorial, Geometric and Alebraic Properies of Quantum Entanglement,” Katholieke Universiteit Leuven, Belgium, July 2004.

L. Gurvits, “Combinatorics Hidden in Hyperbolic Polynomials and Related Topics,” in Proceedings of the 16th International Symposium on Mathematical Theory of Networks and Systems, Belgium, 2004.

L. Gurvits, “Combinatorics Hidden in Hyperbolic Polynomials,” Ireland National University, July 2004.

L. Gurvits, “Convex Geometry of Quantum Entanglement,” SQuInT 2005, Tucson, Ariz., February 2005.

L. Gurvits, “Hyperbolic Rado Theorem,” MSRI (Berkeley), March 2004.

L. Gurvits, "New Lower and Upper Bounds on the Size of Largest Multipartite Separable Ball,” Institute for Quantum Computing, Waterloo, Canada, October 2004. Also given at UCLA in February 2005.

L. Gurvits, “Stability of Positive Switched Systems,” ETH, Zurich, Switzerland, July 2004.

L.Gurvits, “Van der Waerden Conjecture for Mixed Discriminants,” International Algebraic Conference, Moscow, Russia, 2004. Also given at the Moscow State University 250th Anniversary Conference, June 2004.

L.Gurvits, R.Shorten, O.Mason, “Preliminary Results on the Stability of Switched Positive Linear Systems,” in Proceedings of the 16th International Symposium on Mathematical Theory of Networks and Systems, Belgium, 2004.

J. Hogden, R. Brewer, J. Sarracino, M. Cannon, “Blind Inversion of PINEX Data (U),” presented at JOWOG-32M, Aldermaston, U.K. (Also, an internal report, LA-CP-04-0366, Los Alamos National Laboratory.)

A. Hoisie and D. Kerbyson, “A Practical Approach to Performance Analysis and Modeling of Large-Scale Systems,” full-day tutorial, IEEE/ACM SuperComputing, Pittsburgh, Pa., November 2004.

S. Jiang, F. Chen, X. Zhang, “CLOCK-Pro: An Effective Improvement of the CLOCK Replacement,” in Proceedings of the 2005 USENIX Annual Technical Conference USENIX'05, Anaheim, Calif., pp. 87-100, April 2005.

C. Joslyn, “Management of Quantified Semantic Taxonomies for Biothreat Response,” DIMACS Tutorial and Working Group on Order Theoretic Aspects of Epidemiology.

C. Joslyn, “Order Theoretical Knowledge Discovery,” in DIMACS Workshop on Applications of Order Theory to Homeland Defense and Computer Security. (Also, a technical report, LA-UR-04-6208, Los Alamos National Laboratory.)

C. Joslyn, “Reports on Two Recent Bio-Ontology Workshops,” in Proceedings of the Seventh Annual Bio-Ontologies Meeting, ISMB ’04.

C. Joslyn, W. Buehring, P. Kaplan, and D. Powell, “Critical Infrastructure Protection Decision Support System (CIP/DSS): Addressing Uncertainty and Risk,” technical report, LA-UR-04-6720, Los Alamos National Laboratory.

C. Joslyn, J. Cohn, S. Mniszewski, and K. Verspoor, “Order Theoretical Approaches to Automated Functional Annotation Using Bio-Ontologies,” Integrated Biosciences Virtual Seminar on Genomics and Bioinformatics, virtualgenomics.org, November 2004.

C. Joslyn and S. Ferson, “Approximate Representations of Random Intervals for Hybrid Uncertainty Quantification,” in Sensitivity Analysis of Model Output (SAMO04), K. Hanson and F. Hemez (editors), pp. 453-469, Los Alamos National Laboratory, http://library.lanl.gov/cgi-bin/getdoc?event=SAMO2004&document=samo04-83.pdf

C. Joslyn, S. Mniszewski, A. Fulmer, and G. Heaton, “The Gene Ontology Categorizer, Intelligent Systems for Molecular Biology (ISMB 2004),” a technical report, LA-UR-04-0354, August 2004.

C. Joslyn, S. Mniszewski, and K. Verspoor, “Combinatorial Knowledge Discovery for Bio-Ontology Management,” Stanford Medical Informatics.

C. Joslyn, S. Mniszewski, K. Verspoor, and J. Cohn, “Improved Order Theoretical Techniques for GO Functional Annotation,” poster to be presented at Intelligent Systems for Molecular Biology (ISMB 2005), March 2005.

D. Kerbyson, “Comparing Systems Using Application Performance Models,” Cray Advanced Technical Workshop, Bologna, Italy, June 2004.

D. Kerbyson, “Performance Modeling of Large-Scale Systems in PERCS: A Methodology Description,” IBM PERCS Project, July 2004.

D. Kerbyson, M. Lang, G. Patino, H. Amidi, “An Empirical Performance Analysis of Commodity Memories in Commodity Servers,” in Proceedings of the ACM Workshop on Memory System Performance, Washington, D.C., June 2004.

*W. Klein, N. Gulbahce, H. Gould, J. Rundle, and K. Tiampo, “Structure of Fluctuations at Mean-Field and Spino Dal Critical Points,” in preparation.

*Statistical Physics Days, June 24 - 26, 2004, Istanbul, Turkey. Contributed talk: “Quench depth and range of interaction effects in homogeneous and heterogeneous nucleation.”

*Sixth Annual Greater Boston Area Statistical Mechanics Meeting, Oct 16, 2004, Brandeis University, MA. Contributed talk: “Quench depth and range of interaction effects in homogeneous and heterogeneous nucleation.”

*APS March Meeting, Los Angeles, March 20-25, 2005. Contributed talk: “Heterogeneity in classical and non-classical nucleation.”

V. Krishnamurthy, M. Faloutsos, M. Chrobak, L. Lao, J. Cui, and A. Percus, "Reducing Large Internet Topologies for Faster Simulations," in Proceedings of Networking 2005, Waterloo, Ontario, May 2-6, 2005.

M. Mathis and D. Kerbyson, “Performance and Scalability of Particle Transport Calculations,” poster presentation, Department of Energy High Speed Computing Conference, Newport Beach, Ore., April 2004.

M. Mathis and D. Kerbyson, “Performance Modeling of Unstructured Mesh Particle Transport Computations,” in Proceedings of the Workshop on Performance Modeling Evaluation and Optimization (PMEO), Int. Parallel and Distributed Processing Symposium (IPDPS), Santa Fe, N.M., April 2004.

K. Muske, J. Jones, and J. Howse, “Model-Based Fault Detection for Three-Way Automotive Catalyst Systems,” in the Proceedings of the First IFAC Symposium on Advances in Automotive Control, Salerno, Italy, pp. 374-379, April 2004.

S. Pakin, “coNCePTuaL: A Network Correctness and Performance Testing Language,” in Proceedings of the International Parallel and Distributed Processing Symposium (IPDPS 2004), Santa Fe, N.M., April 28-30, 2004. Available at http://www.c3.lanl.gov/~pakin/papers/ipdps2004.pdf.

S. Pakin, “Rapid Development of Application-Specific Network Performance Tests,” to appear in the Proceedings of the International Conference on Computational Science (ICCS 2005), Workshop on Tools for Program Development and Analysis in Computational Science, Atlanta, Georgia, May 22-25, 2005. (Also, a technical paper, LA-UR-05-0275, Los Alamos National Laboratory.) Available at: http://www.c3.lanl.gov/~pakin/papers/tpdacs2005.pdf.

S. Pakin, “Reproducible Network Benchmarks with conceptual,” in Proceedings of Euro-Par 2004, Pisa, Italy, August 31-September 3, 2004. (Also, a technical report, LA-UR-04-6067, Los Alamos National Laboratory.) Available at http://www.c3.lanl.gov/~pakin/papers/europar2004.pdf.

A. Percus, G. Istrate, and C. Moore (editors), “*Computational Complexity and Statistical Physics,”* Oxford University Press, New York, 2005.

A. Percus, G. Istrate, and C. Moore, "Where Statistical Physics Meets Computation," in a forthcoming book, Computational Complexity and Statistical Physics, in production, 2005.

M. Pernice, “Performance of a Newton-Krylov-FAC Method for Equilibrium Radiation Diffusion on Locally Refined Grids,” Eighth Copper Mountain Conference on Iterative Methods, April 2004.

M. Pernice, “Solution of a Streamfunction-Vorticity Formulation of Resistive Magnetohydrodynamics Using Implicit Adaptive Mesh Refinement,” 16th International Conference on Domain Decomposition Methods, January 2005.

F. Petrini, “A Network Operating System for Large-Scale Parallel Machines,” Emory University, Atlanta, Ga.

F. Petrini, “HPCRI (High Performance Computing Reliability Issues), in Conjunction with HPCA (High Performance Computer Architecture),” San Francisco, Calif.

F. Petrini, “System-Level Fault-Tolerance in Large-Scale Parallel Machines with Buffered Coscheduling (Keynote Speech),” Ninth IEEE Workshop on Fault-Tolerant Parallel, Distributed and Network-Centric Systems (FTPDS04), Santa Fe, N.M.

F. Petrini, K. Davis, and J. Sancho, “System-Level Fault-Tolerance in Large-Scale Parallel Machines with Buffered Coscheduling,” in Ninth IEEE Workshop on Fault-Tolerant Parallel, Distributed and Network-Centric Systems (FTPDS04), Santa Fe, N.M., April 2004.

J. Sancho, F. Petrini, K. Davis, R. Gioiosa, and S. Jiang, First Workshop on System Management Tools for Large-Scale Parallel Systems, 19th International Parallel and Distributed Processing Symposium (IPDPS 2005), Denver, Colo., April 2005.

J. Sancho, A. Robles, P. Lopez, J. Flich, and J. Duato, "Performance Evaluation of COWs under Real Parallel Applications," in Proceedings of the Workshop on Communication Architecture for Clusters (CAC'03), April 22, 2003, Nice, France.

J. Sancho, A. Robles, P. Lopez, J. Flich, and J. Duato, "Routing in InfiniBand Torus Network Topologies," in Proceedings of the International Conference on Parallel Processing (ICPP'03), October 6-9, 2003, Kaohsiung, Taiwan.

E. Springer, E. Vivoni, K. Costigan, S. Mniszewski, G. Zyvoloski, P. Fasel, and G. Langhorst, "SAHRA Fine Resolution Model—Status and Needs," Sustainability of Semi-Arid Hydrology and Riparian Areas (SAHRA) Fourth Annual Meeting, October 2004.

I. Steinwart, D. Hush, and C. Scovel, "Fast Rates to Bayes for Kernel Methods," Neural Information Processing Systems (reviewed conference), 2004, in press.

I. Steinwart and C. Scovel, "Anomaly Detection Is Classification," Neural Information Processing Systems (reviewed conference), 2004, in press.

I. Steinwart and C. Scovel, "When Do Support Vector Machines Learn Fast?" 16th International Symposium on Mathematical Theory of Networks and Systems 2004, invited paper with talk. Also given (with variations) at: University of Dortmund, Germany, 2004; University of Bochum, Germany, 2004; Max-Planck Institute for Biological Cybernetics, Tuebingen, Germany, 2004; AMS regional meeting, Albuquerque, N.M., 2004; PASCAL Workshop, Eindhoven, the Netherlands, 2004; 16th International Symposium on Mathematical Theory of Networks and Systems, Leuven, Belgium, 2004; LANL, 2004.

Z. Toroczkai, M. Anghel, G. Korniss, and K. Bassler, "Effects of Inter-Agent Communications on the Collective," in Collectives and the Design of Complex Systems, K. Tumer and D. Wolpert (editors), Springer, 2004.

K. Verspoor, J. Cohn, C. Joslyn, S. Mniszewski, A. Rechtsteiner, L. Rocha, and T. Simas, "The LANL BioCreative Task 2 Submission," poster at Intelligent Systems for Molecular Biology (ISMB 2004), August 2004.

K. Verspoor, J. Cohn, C. Joslyn, S. Mniszewski, A. Rechtsteiner, L. Rocha, and T. Simas, "Protein Annotation as Term Categorization in the Gene Ontology," Biocreative Workshop. (Also, a technical report, LA-UR-04-1460, Los Alamos National Laboratory.)

K. Verspoor, J. Cohn, S. Mniszewski, and C. Joslyn, "Nearest Neighbor Categorization for CASP Function Prediction," poster to be presented at Intelligent Systems for Molecular Biology (ISMB 2005), March 2005.

K. Verspoor, J. Cohn, S. Mniszewski, and C. Joslyn, "Nearest Neighborhood Categorization for Function Prediction," in the Proceedings of the Fifth Community-Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction (CASP 05), in press.

K. Verspoor, J. Cohn, S. Mniszewski, and C. Joslyn, "Nearest Neighbor Categorization for Function Prediction," in Proceedings of the Sixth Community-Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction," Gaeta, Italy. December 4-8. (Also, a technical report, LA-UR-04-7477, Los Alamos National Laboratory.)

T. Warnock, "A Shape Metric Based on the Line Scan Transform," a talk at the Nuclear Explosives Code Developers Conference (NECDC).

T. Warnock, "Statistical Methods for Analysis and Anomaly Detection in Large Hydrocode Datasets," a talk at the Nuclear Explosives Code Developers Conference (NECDC).

Media

K. Patch, "Agent Model Yields Leadership," *Technology Research News*, September 22/29, 2004, text available at:
www.trnmag.com/Stories/2004/092204/Agent_model_yields_leadership_092204.html

Research in Progress

S. Pakin, "The Design and Implementation of a Domain-Specific Language for Network Performance Testing," submitted to the 14th International Conference on Parallel Architectures and Compilation Techniques (PACT-2005).

L. Gurvits, a classical black-box approach to search problems with the same complexity bounds as in Lov Grover's quantum algorithm, 2005.

L. Gurvits, "On the Complexity of Mixed Discriminants and Related Problems," 2005.

L. Gurvits and H. Barnum, "Further Results on the Multipartite Separable Ball," see http://xxx.lanl.gov/abs/quant-ph/0409095. 2004.

L. Gurvits and H. Barnum, "Revisiting Separability of 2\2 Quantum Systems," a paper dealing with the quaternionic approach to quantum separability, 2005.

L. Gurvits and A. Samorodnitsky, "A Note on Common Quadratics Lyapunov Functions for Linear Inclusions: Exact Results and Open Problems," technical report, LA-UR-05-1937, Los Alamos National Laboratory.

B. Philip and M. Pernice, "Performance of FAC Preconditioners for Multi-Material Equilibrium Radiation Diffusion on Adaptively Refined Grids."

B. Philip, M. Pernice, and L. Chacon, "Solution of Reduced Resistive Magnetohydrodynamics Using Implicit Adaptive Mesh Refinement."

Software

S. Pakin released coNCePTuaL on August 24, 2004, LA-CC-03-099. Available from http://conceptual.sourceforge.net/.

Awards

Several staff members in CCS-3 received the Defense Programs Award of Excellence for work done by the ASCI Lightning Integration Team, October 2004.

Computational Biology (CB) Team

L. Bettencourt, A. Cintron-Arias, D. Kaiser, and C. Castillo-Chavez, "The Power of a Good Idea: Quantitative Modeling of the Spread of Ideas from Epidemiological Models," submitted to *PRE*.

L. Bettencourt, J. Lobo, and D. Strumsky, "Innovation in the City: Increasing Returns to Scale in Metropolitan Patenting," submitted to *Research Policy*.

M. Dunlop and M. Wall, "Robustness in Gene Circuits: Clustering of Functional Responses," *Proceedings of the 24th American Control Conference*, in press.

L. Gomes, R. Almeida, L. Bettencourt, V. Almeida, and J. Almeida, "Comparative Graph Theoretical Characterization of Networks of Spam and Legitimate E-Mail," submitted to CEAS05 conference.

L. Gomes, R. Almeida, L. Bettencourt, V. Almeida, and J. Almeida, "Improving Spam Detection Based on Structural Similarity," submitted to *ACM Transactions on Information and System Security (TISSEC)*.

D. Ming and M. Wall, "Quantifying Allosteric Effects in Proteins," *Proteins*, published online, April 8, 2005.

M. Wall, M. Dunlop, and W. Hlavacek, "Multiple Functions of a Feed-Forward-Loop Gene Circuit," *J Mol Biol*, in press.